NEUTRON INDUCED REACTION CROSS-SECTION CALCULATIONS AND GEANT4 SIMULATION FOR THE FUSION REACTOR MATERIAL SiO_2

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Silicon dioxide, also known as silica (from the Latin silex), is a chemical compound that is an oxide of silicon with the chemical formula SiO_2, which has been known since ancient times. Silica is most commonly found in nature as quartz, as well as in various living organisms. Among many areas of its usage, with the developed technology and improved science, it is also considered to be used as fusion reactor material. The material is generally known due to its dielectrically properties. As it's known, for various applications in the field of reactor design and neutron effect, reaction cross–section data are required. The cross–sections of (n,α), (n,p), (n, γ), (n,EL), (n,inEL) and (n,TOT) reactions for ^{28}Si and ^{16}O nuclei have been calculated by using TALYS 1.8 Two Component Exciton model and EMPIRE 3.2 Exciton model in this study. Also, theoretical nuclear reaction cross-section computations have been done with GEANT4 for the SiO_2 for neutron induced reactions. Obtained results from performed calculations were compared with the experimental nuclear reaction data exist in EXFOR.

Introduction

Silicon dioxide (SiO_2) is a technologically important material, which is suitable to be used in many fields such as optics, microelectronics, and the creation of functional and structural materials etc. It also has applications in space technology, primarily for the radiation-protective glass covers of solar batteries. Silica is promising for use as a pigment/filler for thermal-control coatings of spacecraft's [1]. Silicon dioxide has a great number of outstanding chemical and physical properties that provide it a wide range use on potential applications in semiconductor and nuclear industries. For instance, it has been proposed as a structural component in fusion reactors. Therefore, a fundamental understanding of the radiation effects on SiO_2 is needed to be obtained for improving the usage of this material in suggested technological areas.

Increase of modern daily life's energy request with the improvements in technology, cause day-by-day growing energy production. Conventional energy production methods will not be able to cover the request of growing energy demand in clean and safe way. To solve this problem, scientists are still working on one of the possible solutions which is fusion reactors. For a safe design, the development of structural materials and materials microstructure change under the effect of radiation have a great importance. Among many identifiers of a nuclear reaction, cross-section data, which express the possibility of the investigated reactions occurrence have almost vital importance to be able to protect ourselves and study environment from potentially unexpected radiation and its damage.

For fusion reactor technology and its development; neutron induced reaction cross-sections data have a critical importance. Evaluated values in nuclear databases form the cross-section data, which are used to understand the neutron interactions [2]. Material analysis is the basis of reactor design and it depends on the calculated reaction cross-section data via many theoretical and experimental ways. Besides, in addition to the importance of the calculated reaction cross-section data, it is also important even critical to simulate the events and environment on and over the desired material or part of the reactor structure. Since it is unavailable to be able to work on a real working fusion reactor, simulation of the environment and events are become more needed and important.

As a result of all mentioned above, the reaction cross–sections for ^{28}Si and ^{16}O have been calculated. To complete the calculations, TALYS 1.8 [3] and EMPIRE 3.2 [4] codes for neutron induce reaction have been employed. In addition, by using Geant4 [5] the total, elastic and inelastic reaction cross-sections for SiO_2 material have been calculated. Obtained results and related experimental data taken from Experimental Nuclear Reaction Data Library, EXFOR [6] for the studied reactions have been compared with each other and an evaluated nuclear data library, which is TENDL [7].

Calculation Methods

TALYS is a nuclear reaction calculation code for the analysis and estimation of nuclear reactions in the energy range of 1 eV – 1 GeV. The default cross–section calculations were considered by the Two Component Exciton (TCE) model. The proton and neutron type of the produced particles and holes are clearly followed during the reaction in the two–component exciton model [3].

Like TALYS, another code is EMPIRE which has been developed to perform nuclear reaction calculations based on nuclear reaction models over a large range of energies from resonance region keV to several hundreds of MeV and different incident particles [4]. The Empire 3.2 contains the mechanism of pre–equilibrium theoretical nuclear reaction model [8] which dependents on the master equation solution in the form recommended by Cline [9] and Ribansky et al. [10].

GEANT4 is a freely distributed simulation and calculation code, which could be run on Unix based operating systems. Investigation of high-energy physics, medical physics, space and radiation physics are some of the possible usage areas of this widely used code. GEANT4 is an abundant set of physics models to handle the interactions of particles with and inside matter across a very large energy range [5, 11].

Discussions

In this study, reaction cross-sections of $^{28}Si(n,\alpha)^{25}Mg$, $^{28}Si(n,p)^{28}Al$, $^{28}Si(n,\gamma)^{29}Si$, $^{28}Si(n,EL)$, $^{28}Si(n,inEL)$, $^{28}Si(n,TOT)$ and $^{16}O(n,\alpha)^{13}C$, $^{16}O(n,p)^{16}N$, $^{16}O(n,\gamma)^{17}O$, $^{16}O(n,EL)$, $^{16}O(n,inEL)$, $^{16}O(n,TOT)$ have been calculated with TCE and Exciton models from TALYS 1.8 and EMPIRE 3.2 codes, respectively. Also, by using Geant4 $SiO_2(n,EL)$, $SiO_2(n,inEL)$ and $SiO_2(n,TOT)$ reaction cross-sections have been calculated and obtained results have been compared with each other and comparisons are given in Figs. 1–6.

The TALYS 1.8 TCE results are in agreement with the experimental data up to 8 MeV energy. After this energy, TALYS 1.8 and EMPIRE 3.2 model results give similar results like TENDL-2015 data but they pursue experimental results from above in the neutron energy region of 8-16.5 MeV in Fig. 1(a). For Fig. 1(b), calculated data and TENDL-2015 data are above the experimental results.

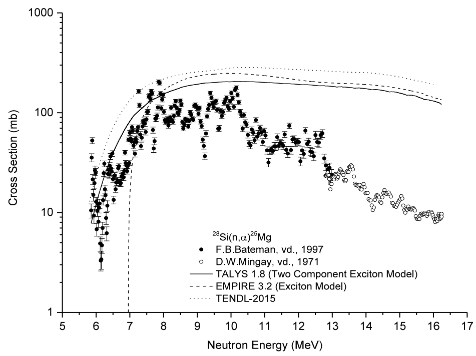

Fig. 1(a). The $^{28}Si(n,\alpha)^{25}Mg$ reaction cross–section calculation

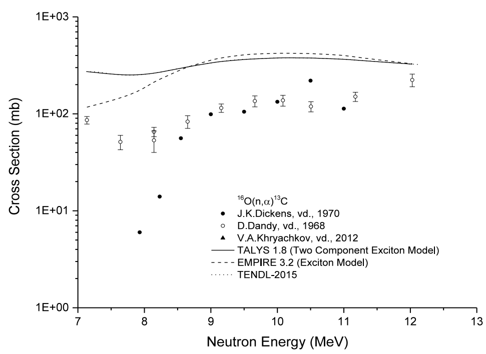

Fig. 1(b). The $^{16}O(n,\alpha)^{13}C$ reaction cross–section calculation

TALYS 1.8 TCE model computations and TENDL-2015 data for $^{28}Si(n,p)^{28}Al$ reaction are almost the same with the experimental results for all investigated energy regions. However, the EMPIRE 3.2 Exciton model was able to compute after 7 MeV neutron energy. Greater than this energy, EMPIRE 3.2 and TALYS 1.8 model results are almost in the same shape given as Fig. 2(a). The all model results were able to obtained after 13.5 MeV neutron energy. TALYS 1.8 TCE model and TENDL-2015 data results are in agreement with the experimental data. EMPIRE 3.2 model results fallow the experimental data from bellow in the neutron energy region of 16-19 MeV shown as Fig. 2(b).

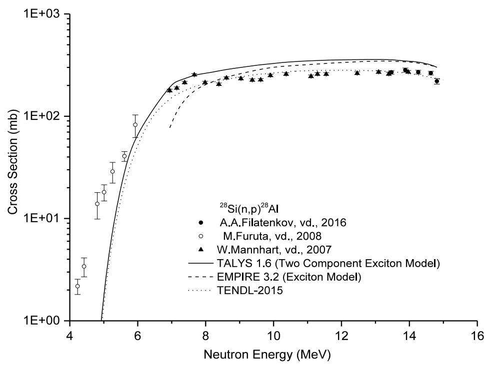

Fig. 2(a). The $^{28}Si(n,p)^{28}Al$ reaction cross–section calculation

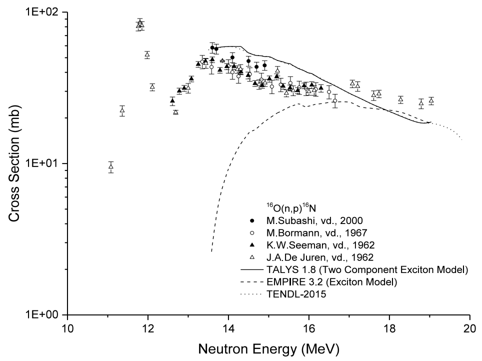

Fig. 2(b). The $^{16}O(n,p)^{16}N$ reaction cross–section calculation

In all studied neutron induced energy region for $^{28}Si(n,\gamma)^{29}Si$ reaction, obtained results have been given in Fig. 3(a). As it can be seen from the figure between 2.5-10 MeV neutron energy region TALYS results are in the agreement with experimental data.
Since the Oxygen is a light weight element and the experimental data for $^{16}O(n,\gamma)^{17}O$ reaction were at low energy region the obtained results for this reaction via TALYS and EMPIRE codes have been totally in disagreement with the experimental data represented as in Fig. 3(b).

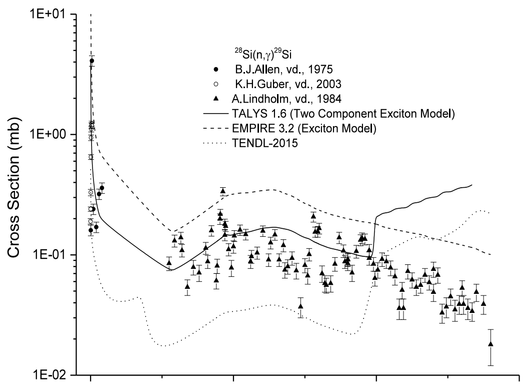

Fig. 3(a). The $^{28}Si(n,\gamma)^{29}Si$ reaction cross–section calculation

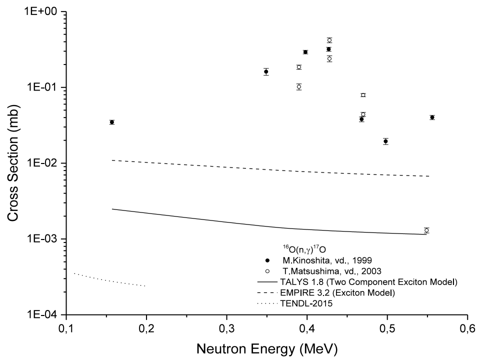

Fig. 3(b). The $^{16}O(n,\gamma)^{17}O$ reaction cross–section calculation

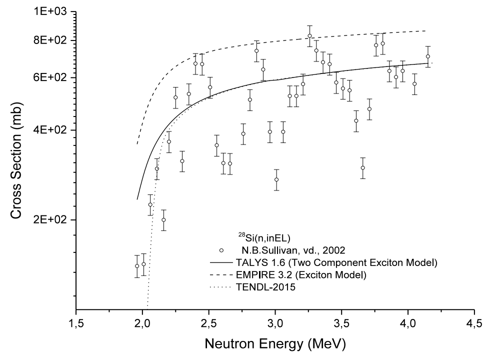

Fig. 5(a). The $^{28}Si(n,inEL)$ reaction cross–section calculation

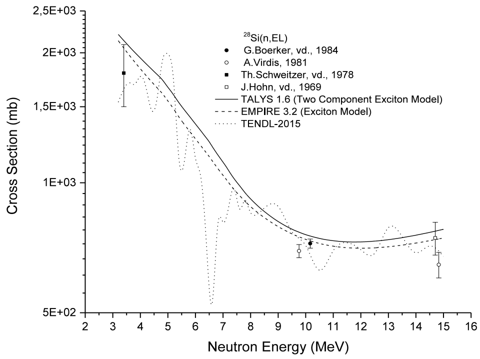

Fig. 4(a). The $^{28}Si(n,EL)$ reaction cross–section calculation

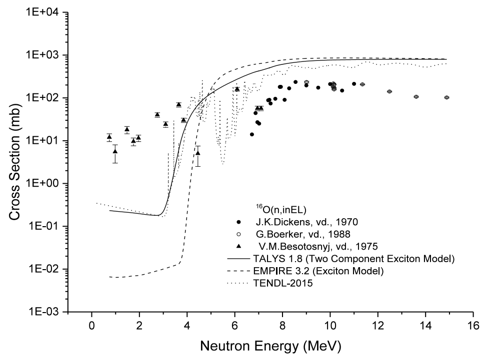

Fig. 5(b). The $^{16}O(n,inEL)$ reaction cross–section calculation

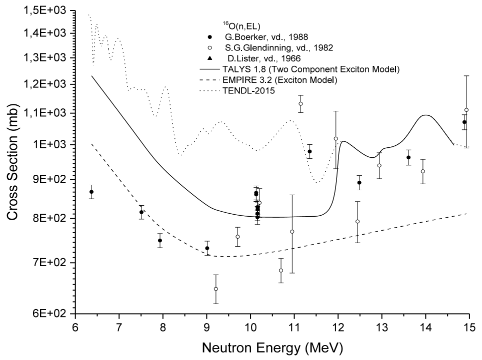

Fig. 4(b). The $^{16}O(n,EL)$ reaction cross–section calculation

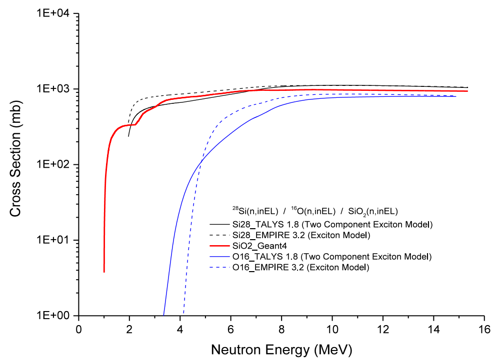

Fig. 5(c). The $SiO_2(n,inEL)$ reaction cross–section calculation

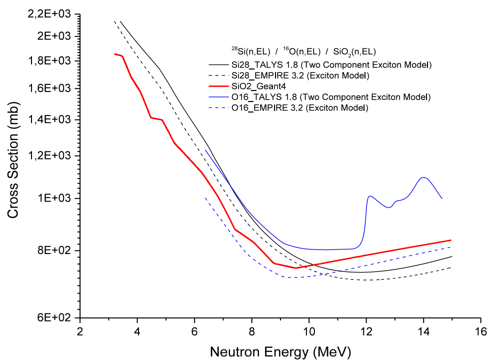

Fig. 4(c). The $SiO_2(n,EL)$ reaction cross–section calculation

The comparisons for $^{28}Si(n,EL)$, $^{16}O(n,EL)$ and $SiO_2(n,EL)$ reactions have been given in Fig. 4(a, b, c) respectively while the comparisons for $^{28}Si(n,inEL)$, $^{16}O(n,inEL)$ and $SiO_2(n,inEL)$ reactions have been given in Fig. 5(a, b, c) respectively. Considering all calculations completed with TALYS and EMPIRE for previously mentioned reactions, TALYS results have more agreement with the EXFOR data rather than EMPIRE results. Results obtained from GEANT4, which employed to observe the cross-sections of SiO_2 material, for elastic and ineleastic reactions are given in Fig. 4(c) and Fig. 5(c) where the agreement between theoretical calculation model results are observable.

The last reaction investigated in this study was the total cross-section reaction for neutron induced particle on ^{28}Si, ^{16}O and SiO_2. When the results were examined; the $^{28}Si(n,TOT)$ reaction cross-section results were above the $SiO_2(n,TOT)$ reaction cross-section and the $^{16}O(n,TOT)$ reaction cross- section

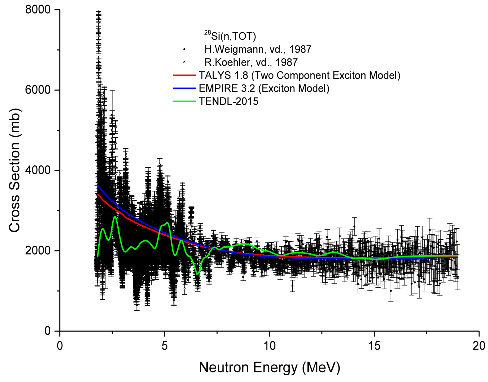

Fig. 6(a). The ^{28}Si(n,TOT) reaction cross–section calculation

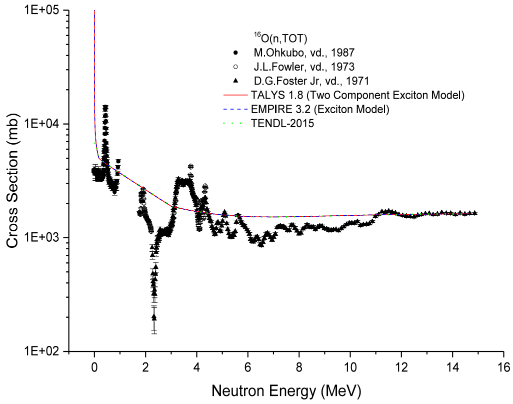

Fig. 6(b). The ^{16}O(n,TOT) reaction cross–section calculation

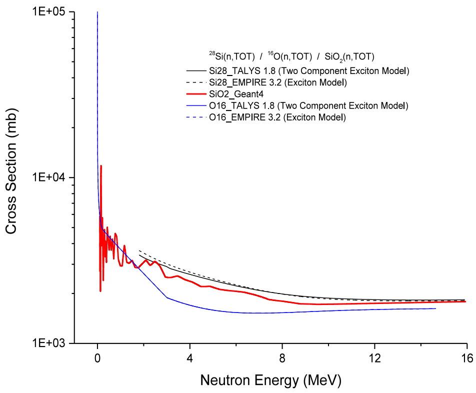

Fig. 6(c). The SiO_2(n,TOT) reaction cross–section calculation

values were below the SiO_2 reaction cross-section.

Conclusion

The TALYS 1.8 Two Component Exciton model computations give similar results with experimental values for almost all reactions. On the other hand, EMPIRE 3.2 Exciton model computations are in agreement with the experimental results for elastic and inelastic reaction cross-section on both ^{28}Si and ^{16}O. The reaction cross-section computations for (n,TOT) reactions obtained via employed models for selected isotopes almost have the same results with the experimental values.

As it can be seen from the (n,TOT) reaction graphs, the reaction cross-section values decrease with the increase of induce particle energy and for SiO2 material the total cross-section values on the neutron induced reactions have an acceptable rate to be used in many applications.

Comparisons show that, in the absence of experimental results, TALYS for isotopes, and GEANT4 for compounds could be usable.

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